

# Improved Density Functionals for Water

Donald G. Truhlar, University of Minnesota

ITR-0428774

The ubiquitous nature of water has prompted great interest in using simulation techniques, such as molecular dynamics and Monte Carlo methods, to better understand the structure and properties of liquid water and ice. Recent attention has focused on using density functional theory (DFT) as a means to study these systems, however the high expense of these simulations has restricted the choice of available density functionals to less costly, and often, less accurate, methods.

We have compared a series of 25 density functional methods to highly accurate *ab initio* data for a set of 28 water dimers and 8 water trimers, in order to assess the accuracy of existing density functional methods. Furthermore, we have gone on to optimize a new functional, PBE1W, that achieves accuracy equal to that of the best existing (and more costly DFT methods) while retaining the cost-effectiveness of those methods currently in use.

